

Claims ART 21 AMDT

1. An organometallic compound of formula $RO-M(L^1)_x(L^2)_y(L^3)_z$

wherein M is a metal selected from titanium, zirconium, hafnium, iron (III), cobalt (III) or aluminium;

R is alkyl or a hydroxy-alkyl, hydroxyalkoxyalkyl, or (hydroxy)polyoxyalkyl group, and

(i) when R is alkyl, L^1 and L^2 are each independently selected from a β -diketonate, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof or siloxy,

(ii) when R is a hydroxy-alkyl hydroxyalkoxyalkyl, or (hydroxy)polyoxyalkyl group, L^1 and L^2 are each independently selected from a diketonate, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof, R^1COO^- where R^1 is substituted or unsubstituted $C_1 - C_{30}$ branched or linear alkyl, substituted or unsubstituted aryl including polycyclic structures such as naphthyl or anthracyl, phosphate, phosphinate, phosphonate, siloxy or sulphonato;

in both case (i) and case(ii), provided that when L^1 is a ligand which forms two covalent bonds with the metal atom, and $x = 1$ then $y = 0$;

L^3 is selected from substituted or unsubstituted phenol or naphthol, R^2COO^- where R^2 is a linear or branched $C_1 - C_{30}$ alkyl or benzene, a polyoxyalkoxy or hydroxyalkoxyalkoxy group;

x and y are each either 0 or 1,

z=1

$(x+y+z) \leq V-1$, where V= the valency of the metal M.

2. An organometallic compound according to claim 1, wherein R is a $C_1 - C_8$ alkyl group or a hydroxy-alkyl group derived from a diol.

3. An organometallic compound according to claim 2, wherein R is selected from the group consisting of ethyl, n-propyl, isopropyl, n-butyl, t-butyl, pentyl, hexyl, hydroxybutyl, polyoxyethyl and 2-(2-hydroxyethoxy)-ethyl.

4. An organometallic compound according to any one of claims 1 – 3, wherein L^1 and L^2 are selected from acetyl acetone, an alkylacetoacetate, an N-alkylacetoacetamide, salicylic acid or ester thereof, mandelic acid or ester thereof, levulinic acid or ester thereof, or naphthalene dicarboxylic acid or ester thereof,

5. An organometallic compound according to any one of claims 1 – 4, wherein L^3 is selected from the group consisting of substituted or unsubstituted phenol or naphthol, or a $C_2 - C_{30}$ carboxylic acid.

6. A cure catalyst composition, suitable for catalysing the formation of urethane bonds, comprising a mixture of an organometallic compound according to any one of claims 1 – 5 and an acid.

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7. A cure catalyst composition according to claim 6, wherein said organometallic compound and said acid are mixed together in a mole ratio of from 0.1 to 10 moles of acid per mole of organometallic compound.

8. A cure catalyst composition according to either claim 6 or claim 7, wherein the acid is a C_2 - C_{30} carboxylic acid.

9. A composition comprising:

a) either

- i) a compound having more than one hydroxy group which is capable of reacting with an isocyanate group-containing material to form a polyurethane or
- ii) a compound having more than one isocyanate group which is capable of reacting with a hydroxyl group-containing material to form a polyurethane,

b) an organometallic compound of formula $RO-M(L^1)_x(L^2)_y(L^3)_z$

wherein M is a metal selected from titanium, zirconium, hafnium, iron (III), cobalt (III) or aluminium;

R is alkyl or a hydroxy-alkyl, hydroxyalkoxyalkyl, or (hydroxy)polyoxyalkyl group, and

(i) when R is alkyl, L^1 and L^2 are each independently selected from a β -diketonate, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof or siloxy,

(ii) when R is a hydroxy-alkyl hydroxyalkoxyalkyl, or (hydroxy)polyoxyalkyl group, L^1 and L^2 are each independently selected from a diketonate, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof, R^1COO- where R^1 is substituted or unsubstituted $C_1 - C_{30}$ branched or linear alkyl, substituted or unsubstituted aryl including polycyclic structures such as naphthyl or anthracyl, phosphate, phosphinate, phosphonate, siloxy or sulphonato;

in both case (i) and case(ii), provided that when L^1 is a ligand which forms two covalent bonds with the metal atom, and $x = 1$ then $y = 0$;

L^3 is selected from substituted or unsubstituted phenol or naphthol, R^2COO- where R^2 is a linear or branched $C_1 - C_{30}$ alkyl or benzene, a polyoxyalkoxy or hydroxyalkoxyalkoxy group;

x and y are each either 0 or 1,

z=1

$(x+y+z) \leq V-1$, where V= the valency of the metal M; and optionally

c) one or more further components selected from chain modifiers, diluents, flame retardants, blowing agents, release agents, water, coupling agents, lignocellulosic preserving agents, fungicides, waxes, sizing agents, fillers, colourants, impact modifiers, surfactants, thixotropic agents, flame retardants, plasticisers, and other binders.

10. A composition according to claim 9, wherein when R is alkyl, L¹ and L² are each independently selected from a β -diketonate, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof, or siloxy.

11. A composition according to claim 10, further comprising an acid.

12. A composition according to claim 11, wherein the acid is intimately mixed with the organometallic compound of component b).

13. A composition according to claim 11, wherein the acid is a C₂ – C₃₀ carboxylic acid.

14. A process for manufacturing an organometallic composition, comprising reacting together:-

(a) a metal alkoxide, having a formula M(OR)_V, where:

M is a metal selected from titanium, zirconium, hafnium, iron (III), cobalt (III) or aluminium;

V= the valency of the metal M, and

R is alkyl, and

(b) a β -diketone, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof, R¹COO- where R¹ is substituted or unsubstituted C₁ – C₃₀ branched or linear alkyl, substituted or unsubstituted aryl including polycyclic structures such as naphthyl or anthracyl, phosphate, phosphinate, phosphonate, siloxy or sulphonate; in an amount to provide about 1 or 2 moles of component (b) per mole of metal M in component (a); and

(c) a substituted or unsubstituted aryloxy, R²COO- where R² is a linear or branched C₁ – C₃₀ alkyl or a substituted or unsubstituted aryl; a polyoxyalkylalcohol or hydroxyalkoxyalcohol in an amount to provide about 1 mole of component (c) per mole of metal M in component (a);

(d) optionally removing alcohol ROH formed during the reaction of (a) with (b) and (c).

15. A process as claimed in claim 14 for manufacturing an organometallic compound according to any of claims 1 – 5.

16. A process as claimed in claim 14 or claim 15, wherein the metal alkoxide M(OR)_V is first reacted with one of component (b) or component (c) and then with the other of components (b) or (c) and the alcohol ROH formed during the reaction of the alkoxide with components (b) and (c) is removed after each reaction step.

17. A process as claimed in any of claims 14 to 16, wherein the product is further reacted with a hydroxy-functionalised alcohol which is preferably a hydroxy-alcohol, hydroxyalkoxyalcohol, or (hydroxy)polyoxyalkylalcohol and a further quantity of ROH is removed from the reaction mixture.

18. A process for the manufacture of a polyurethane article, comprising the steps of:

a) forming a mixture by mixing together either

i) a compound having more than one hydroxy group which is capable of reacting with an isocyanate group-containing material to form a polyurethane or

ii) a compound having more than one isocyanate group which is capable of reacting with a hydroxyl group-containing material to form a polyurethane,

with an organometallic compound of formula $RO-M(L^1)_x(L^2)_y(L^3)_z$

wherein M is a metal selected from titanium, zirconium, hafnium, iron (III), cobalt (III) or aluminium;

L^1 and L^2 are each independently selected from a diketone, an ester or amide of acetoacetic acid, a hydroxycarboxylic acid or ester thereof, R^1COO- where R^1 is substituted or unsubstituted $C_5 - C_{30}$ branched or linear alkyl, substituted or unsubstituted aryl including polycyclic structures such as naphthyl or anthracyl, phosphate, phosphinate, phosphonate, siloxy or sulphonato, provided that when L^1 is a ligand which forms two covalent bonds with the metal atom, and $x = 1$ then $y = 0$;

L^3 is selected from substituted or unsubstituted aryloxy, R^2COO- where R^2 is a linear or branched $C_6 - C_{30}$ alkyl, and a polyoxyalkyl or hydroxyalkoxyalkyl group;

R is alkyl or hydroxy-alkyl hydroxyalkoxyalkyl, or (hydroxy)polyoxyalkyl group,

x, y and z are each either 0 or 1

$(x+y+z) \leq V-1$, where V = the valency of the metal M;

b) adding to said mixture the other of the compound having more than one hydroxy group which is capable of reacting with an isocyanate group-containing material to form a polyurethane or the a compound having more than one isocyanate group which is

capable of reacting with a hydroxyl group-containing material to form a polyurethane,

c) forming said mixture into the required shape for the polyurethane article;

d) allowing said mixture to cure

e) optionally subjecting the mixture to specified conditions for post-cure conditioning.